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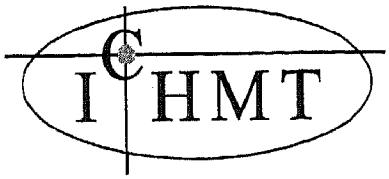

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EVALUATION OF THE SNB BASED FULL-SPECTRUM CK METHOD FOR THERMAL RADIATION CALCULATIONS IN CO_2-H_2O MIXTURES

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ABSTRACT. The statistical narrow-band model based full-spectrum correlated-k method was developed for calculations of thermal radiation in non-isothermal and inhomogeneous CO_2-H_2O-grey particulate mixtures. Two different methods to handle mixtures of CO_2 and H_2O were proposed. The accuracy and efficiency of these two implementations of the statistical narrow-band based full-spectrum correlated-k method for calculations of thermal radiation in CO_2-H_2O-N_2 mixtures were evaluated against the standard statistical narrow-band correlated-k method and the optimized 9-band model in the calculations of two non-isothermal problems in a three-dimensional rectangular enclosure. Results of the first implementation method are slightly more accurate but somewhat less efficient than the optimized 9-band model. The second implementation method is very efficient but is also considerably less accurate.

INTRODUCTION

Development of accurate and efficient models for modelling non-grey radiation from real gases continues to draw considerable research effort. Such models are highly desirable for implementation into multidimensional CFD and flame codes to perform fully coupled calculations of combustion, flame, and other high temperature problems. It has been well recognized that the simple grey gas model, though computationally efficient, in general gives rise to unacceptable errors. Approximate non-grey gas radiation models developed in the last decade or so can be classified into two categories: hybrid models that implement the classical wide-band or statistical narrow-band (SNB) models through the correlated-k (CK) methodology [1-6] and various global models. The latter consists of the spectral-line based weighted-sum-of-grey-gases (SLW) models [7-10], the absorption distribution function (ADF) models [11,12], and the more recently developed full-spectrum correlated-k (FSCK) methods [13-16].

It is worth noting that computational efficiency, solution accuracy, and model capability in general represent competing factors in the development of non-grey gas radiation models. For example, the standard implementation of the SNB based CK method (SNB-CK) for radiation heat transfer calculations [17] offers excellent accuracy and full capability to handle non-grey boundary walls and non-grey absorption, emission, and scattering by particulates, but is still too computationally demanding to be utilized in multidimensional calculations. This is because the radiative transfer equation (RTE) is solved 367 (number of narrow-bands) × M (number of quadrature points) times to obtain the total radiation intensity. On the other hand, global models in general offer relatively good accuracy and excellent efficiency, but are in general unable to deal with non-grey walls and/or non-grey absorption and scattering by particulates. Global models formulated in terms of absorption coefficient distribution, however, suffer from the difficulty of dealing with these non-grey effects since the spectral information is lost as a result of reordering in these models. Although it has been shown by Solovjov and Webb [10] that non-grey absorption and emission by soot can be incorporated into SLW, further extension of SLW to include effects of non-grey walls and non-grey

scattering appears to be very difficult. In general, spectral band models offer the best compromise when dealing with non-grey walls and non-grey particulate. The SNB-CK models developed by Liu et al. [6] are accurate, efficient and capable of dealing with non-grey walls and non-grey particulate and represent a good compromise between accuracy, efficiency, and capability. In addition, the SNB-CK models offer good flexibility due to the fact that the SNB based cumulative absorption coefficient distribution function has an analytical expression.

For calculations in problems where boundary effects are either grey (such as in furnaces) or unimportant (such as in modelling of open flames) and particulates (if any) can be assumed either grey or unimportant, the standard and the modified SNB-CK methods developed so far [5,6,17] are less efficient compared to the FSCK method for the following two reasons. First, the blackbody function at each band is required to be constant in the SNB-CK methods [1,2,5]. This requirement imposes a limitation on the bandwidth of these methods, i.e. their accuracy deteriorates as the bandwidth increases [6]. Secondly, the inversion of the cumulative distribution function consumes a significant portion of the total cpu time. In this study, it is shown that the SNB-CK method can be extended to full-spectrum through the FSCK methodology recently developed by Modest and Zhang [13-16]. Two different approaches to handle mixtures of CO_2 and H_2O were proposed. Besides the advantage of working with the analytical expression of the SNB absorption coefficient distribution function, another important consideration for developing SNB-FSCK methods is that the recent SNB model parameters compiled by Soufiani and Taine [18] were found to predict transmissivity of CO_2 at high temperatures in better agreement with experimental measurements than that predicted using HITEMP database [19]. The SNB-FSCK methods developed in this study were evaluated against the standard SNB-CK method [17] and the recently developed optimized 9-band model [20] in terms of efficiency and accuracy in the calculations of radiation heat transfer in a three-dimensional rectangular enclosure containing non-isothermal and inhomogeneous CO_2-H_2O-N_2 mixtures. The inclusion of grey particulates in the SNB-FSCK methods is straightforward. Therefore, numerical results with grey particulates are not presented due to space limitation.

FORMULATION

SNB-FSCK method The spectral RTE in an absorbing, emitting and scattering medium is written as [21]

$$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu + \kappa_\nu I_{b\nu}(T) - \sigma_\nu I_\nu + \frac{\sigma_\nu}{4\pi}\int_{4\pi} I_\nu(\hat{s}')\Phi_\nu(\hat{s},\hat{s}')d\Omega' \tag{1}$$

It is necessary to assume that scattering properties (scattering coefficient and phase function) and wall properties are grey in any global model [16]. Following the full-spectrum analysis of Modest [16], Eq.(1) can be converted into the following form by first multiplying with $\delta(k-\kappa_\nu(\nu,\underline{\phi}_0))$ followed by integration over the entire spectrum and division by $f(T_0,\underline{\phi}_0,k)$

$$\frac{dI_g}{ds} = k^*(T_0,\underline{\phi},g_0)\left[a(T,T_0,g_0)I_b(T) - I_g\right] - \sigma_s I_g + \frac{\sigma_s}{4\pi}\int_{4\pi} I_g(\hat{s}')\Phi(\hat{s},\hat{s}')d\Omega' \tag{2}$$

provided that at every wavenumber in the entire spectrum where $\kappa_\nu(\nu,\underline{\phi}_0) = k$ there is a unique value for $\kappa_\nu(\nu,\underline{\phi}) = k^*(T_0,\underline{\phi},k)$. In Eq.(2), I_g, f, g_0, and a are defined as

$$I_g = \int_0^\infty I_\nu \delta(k-\kappa_\nu(\nu,\underline{\phi}_0))d\nu / f(T_0,\underline{\phi}_0,k) \tag{3}$$

$$f(T,\underline{\phi}_0,k) = \frac{1}{I_b(T)}\int_0^\infty I_{b\nu}(T)\delta(k-\kappa_\nu(\nu,\underline{\phi}_0))d\nu \tag{4}$$

$$g_0(T_0,\underline{\phi}_0,k) = \int_0^k f(T_0,\underline{\phi}_0,k)dk \tag{5}$$

$$a(T,T_0,g_0) = f(T,\underline{\phi}_0,k)/f(T_0,\underline{\phi}_0,k) \tag{6}$$

Function f is a Planck function weighted full-spectrum absorption coefficient distribution function which depends on the reference state $\underline{\phi}_0$ and the local (the Planck function) temperature T. Using the property of the δ function Eq.(4) can be written as

$$f(T,\underline{\phi}_0,k)=\frac{1}{I_b(T)}\sum_i I_{bvi}(T)\left|\frac{dv}{d\kappa_v}\right|(v_i,\underline{\phi}_0) \tag{7}$$

where the summation is over all the occurrences of $\kappa_v(v,\underline{\phi}_0)=k$. Since $\kappa_v(v,\underline{\phi})=k^*(T_0,\underline{\phi},k)$ is a unique function of $\kappa_v(v,\underline{\phi}_0)=k$, one has [16]

$$f(T,\underline{\phi}_0,k)dk=f(T,\underline{\phi},k^*)dk^* \tag{8}$$

If it is further assumed that $\kappa_v(v,\underline{\phi})$ is a monotonically increasing function of $k=\kappa_v(v,\underline{\phi}_0)$, the following relation is obtained based on the definition of the cumulative distribution function [16]

$$g(T,\underline{\phi}_0,k)=\int_0^k f(T,\underline{\phi}_0,k)dk=\int_0^{k^*} f(T,\phi,k^*)dk^*=g(T,\phi,k^*) \tag{9}$$

Eq.(9) implies that k^* (the absorption coefficient at the actual state $\underline{\phi}$) is inverted from the same g value calculated at a k value determined by the reference state $\underline{\phi}_0$, the reference Planck function temperature T_0, and a pre-defined g value g_0, i.e. k is inverted from Eq.(5).

The SNB-FSCK method is formulated by realizing that the integration over the entire spectrum in Eq.(4) can be evaluated as summation of integration over each narrow-band, i.e.

$$f(T,\underline{\phi}_0,k)=\frac{1}{I_b(T)}\sum_{n=1}^{367}\int_{\Delta v} I_{bv,n}(T)\delta(k-\kappa_v(v,\underline{\phi}_0))dv=\frac{1}{I_b(T)}\sum_{n=1}^{367} I_{bv,n}(T)f_{NB,n}(\underline{\phi}_0,k)\Delta v \tag{10}$$

where Δv is the bandwidth of narrow-bands (25 cm^{-1}) and the summation is over 367 narrow-band covering the spectral range of 150 to 9300 cm^{-1} [18]. In Eq.(10), $f_{NB,n}$ is the normalized narrow-band absorption coefficient distribution function and is related to the SNB model through [2,5]

$$f_{NB,n}(\underline{\phi}_0,k)=\frac{1}{2}k^{-3/2}(B_nS_n)^{1/2}\exp\left[\frac{\pi B_n}{4}(2-\frac{S_n}{k}-\frac{k}{S_n})\right] \tag{11}$$

where B_n and S_n are related to the SNB model parameters at the reference state $\underline{\phi}_0$. The cumulative distribution function can also be similarly formulated in terms of the SNB model property as

$$g(T,\underline{\phi}_0,k)=\frac{1}{I_b(T)}\sum_{n=1}^{367} I_{bv,n}(T)g_{NB,n}(\underline{\phi}_0,k)\Delta v \tag{12}$$

where $g_{NB,n}$ is the SNB cumulative distribution function given as [2,5]

$$g_{NB,n}(\phi_0,k)=\frac{1}{2}\left[1-\mathrm{erf}(a_n/\sqrt{k}-b_n\sqrt{k})\right]+\frac{1}{2}\left[1-\mathrm{erf}(a_n/\sqrt{k}+b_n\sqrt{k})\right]e^{\pi B_n} \tag{13}$$

where $a_n=0.5\sqrt{\pi B_nS_n}$, $b_n=0.5\sqrt{\pi B_n/S_n}$ and erf is the error function.

To illustrate the solution procedure of the SNB-FSCK method, three cumulative distribution functions of H_2O under the condition of T_0 = 1000 K, T = 1500 K, p = 1 atm and X_{H2O} = 0.2 are plotted in Fig. 1. At a specified numerical quadrature point g_0 = 0.8 (the procedure described below is applicable for any other values), the first step is to invert Eq.(5) with the help of Eqs.(12) and (13) to obtain k. This is indicated in the figure by the arrow line marked 1. The second step is to calculated the new g value, the left hand side of Eq.(9), using the k value from the first step, as illustrated in Fig.1 by the arrow line marked 2. The third step is to invert Eq.(9), the right hand side, again with the help of Eqs.(12) and (13), to obtain k^* as graphically indicated in Fig. 1 by the arrow line marked 3. The fourth step is to calculate the weight function a using Eqs.(6), (10), and (11).

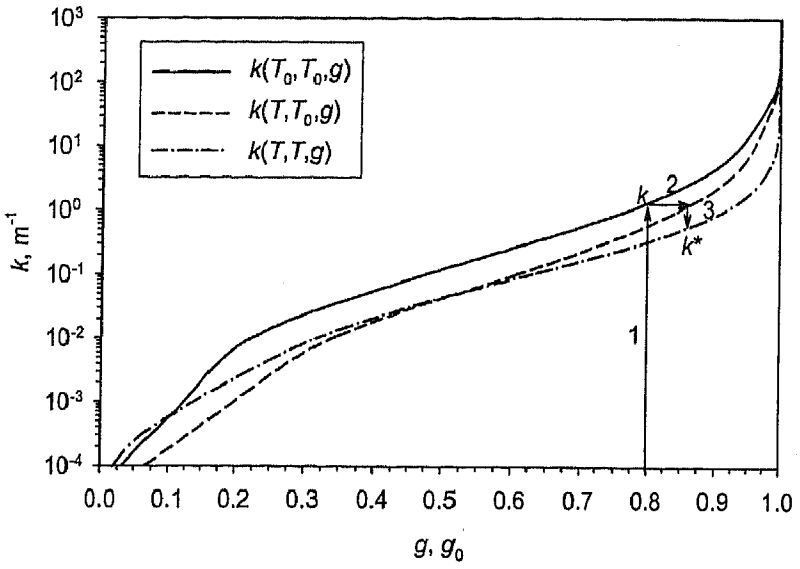

Figure 1. Distributions of correlated absorption coefficients of H_2O

Once a and k^* are obtained, the full-spectrum RTE expressed in Eq.(2) can be solved using any RTE solution technique along with appropriate boundary condition given in [13]. The total radiation intensity is finally evaluated from

$$I = \int_0^1 I_g dg_0 \approx \sum_{i=1}^{M} I_{g_{0i}} w_i \tag{14}$$

The second part of Eq.(14) is an approximation of the integration by a Gauss quadrature scheme defined by M pairs of quadrature points g_{0i} and weight factors w_i.

Treatment of mixtures containing CO_2 and H_2O The solution procedure of the SNB based FSCK method described above can be followed to solve radiation heat transfer problems only with a single radiating species, such as CO_2 or H_2O. Treatment of mixtures of CO_2 and H_2O in general causes difficulties in both band models and global models. It is highly desirable to develop efficient and accurate treatments to handle mixtures of radiating gases, namely CO_2 and H_2O, since these species are almost always simultaneously present in flames or the products of practical hydrocarbon-based combustion systems. Within the present context, the following two methods to deal with mixtures of CO_2 and H_2O are proposed.

The first method (hereafter called M1) is to treat each overlapping narrow-band as an approximate Malkmus band and the approximate band parameters are calculated as [22]

$$S_n = S_{CO_2,n} + S_{H_2O,n} \tag{15}$$

$$B_n = S_n^{\,2} \Big/ \left(\frac{S_{CO_2,n}^{\,2}}{B_{CO_2,n}} + \frac{S_{H_2O,n}^{\,2}}{B_{H_2O,n}} \right) \tag{16}$$

As such, the overlapping narrow-bands become non-overlapping ones and the calculation of both k^* and a described above in the solution procedure of the SNB-FSCK method is applicable for CO_2-H_2O mixtures, with band parameters modified according to Eqs.(15) and (16). In the second method (hereafter called M2), $k^*_{CO_2}$ and $k^*_{H_2O}$ are first separately pre-calculated using the approach described below. It is then assumed that the full-spectrum absorption coefficients of CO_2 and H_2O are correlated. Under this assumption, the absorption coefficient of the mixture k^* at each quadrature point can be simply evaluated as

$$k^* = k^*_{CO_2} + k^*_{H_2O} \tag{17}$$

Pre-calculations of $k^*_{CO_2}$ and $k^*_{H_2O}$ The inversion of Eq.(9) to obtain k^* can consume a significant portion of total cpu time in thermal radiation calculations. In addition, it is not feasible to tabulate k^* at some discrete temperatures since in the SNB based CK methods the inverted absorption coefficients for CO_2-H_2O mixtures depend not only on temperature but also on partial pressures of CO_2 and H_2O. While it is not practical to pre-calculate the absorption coefficients of CO_2-H_2O mixtures in the first method for handling the mixtures, it is possible to pre-calculate the absorption coefficients of CO_2 and H_2O in the second one. Availability of pre-calculated absorption coefficients $k^*_{CO_2}$ and $k^*_{H_2O}$ (for a specified Gauss quadrature scheme) in the second method can make the SNB-FSCK method even more efficient. Our numerical experiments indicate that the values of $k^*_{CO_2} / pX_{CO_2}$ (absorption coefficient per partial pressure) and $k^*_{H_2O} / pX_{H_2O}$ are strongly dependent on the local temperature T and the reference temperature T_0, but otherwise only weakly dependent on the values of the reference mole fractions $X_{CO_2 0}$ and X_{H_2O0}. The reason for such weak dependence is that, as observed by Liu and Smallwood [20], the collision half-width of the absorption lines of radiating gases is weakly dependent on mole fractions of radiating gases. Consequently, it is possible to pre-calculate $k^*_{CO_2} / pX_{CO_2}$ and $k^*_{H_2O} / pX_{H_2O}$ for a chosen reference mixture defined in [20], i.e. $X_{CO_2 0} = 0.1$ and $X_{H_2O0} = 0.2$. For a specified Gauss quadrature scheme and a given reference temperature T_0, $k^*_{CO_2} / pX_{CO_2}$ and $k^*_{H_2O} / pX_{H_2O}$ can be calculated for a range of temperatures. In this study, the values of $k^*_{CO_2} / pX_{CO_2}$ and $k^*_{H_2O} / pX_{H_2O}$ calculated for the 4-point Gauss quadrature scheme were fit accurately to a 9th-order polynomial function of T between 300 and 2600 K at a series of reference temperatures T_0 between 500 and 1600 K (with intervals of 100 K). In applying this method to problems where the actual reference temperature T_0 falls between two neighboring prescribed reference temperatures T_{01} and T_{02}, the actual absorption coefficients are calculated by linear interpolation between those at T_{01} and T_{02}.

RESULTS AND DISCUSSION

The SNB-FSCK methods described above were employed to calculate thermal radiation transfer in a three-dimensional rectangular enclosure containing non-isothermal CO_2-H_2O-N_2 mixtures. The pressure considered is 1 atm. All boundary surfaces are assumed to be black and cold at 0 K. The RTE was solved using DOM with the step spatial differencing scheme and the T_3 angular discretisation scheme. The dimensions of the enclosure are $2m(L_x) \times 2m(L_y) \times 8m(L_z)$. The enclosure is divided into $17(x) \times 17(y) \times 40(z)$ control volumes. The division in x and y directions is uniform. Non-uniform grids are used in the z direction to better resolve the large temperature gradient region. The non-uniform temperature distribution is specified as $T = (T_{axis} - 800) f(r) + 800$ where T_{axis} and $f(r)$ define the temperature distribution along the centerline and radial direction, respectively, with $T_{axis} = 400 + (2100 - 400)z / 0.75$ for $z < 0.75$ m, $T_{axis} = 800 + (2100 - 800)(8 - z) / 7.25$ for $z > 0.75$ m, and $f(r)$ given as $f(r) = 1 - 3r^2 + 2r^3$ (r is the distance to the centerline). In the four corner regions where r is greater than 1 m, T simply takes the value of temperature at r = 1 m. The peak temperature of 2095.5 K occurs along the centerline at z = 0.775 m. A schematic of the enclosure and the temperature distribution in the x-z plane at y = 0 are shown in Fig. 2. The geometry and temperature distribution in these test cases simulate a water-cooled gas-fired furnace. Following the recommendation of Modest and Zhang [13], the reference temperature T_0 is calculated from

$$\left(\kappa_P T^4\right)_0 = \frac{1}{V} \int_V \kappa_P T^4 dV \tag{18}$$

where V is the entire volume of the enclosure and the Planck mean absorption coefficient on the left hand side is calculated at the reference temperature T_0 and the reference mixture defined earlier, i.e. T_0 is obtained iteratively from Eq.(18).

In the following discussions, results obtained from the standard SNB-CK method (bandwidth 25 cm^{-1}) using the 7-point Gauss-type quadrature [22] are used as the benchmark solution. Calculations of the SNB-FSCK methods and the optimized 9-band model with pre-calculated absorption coefficients [20] were conducted using the 4-point Gauss quadrature. All calculations were carried out on a Pentium 4 2.8 GHz PC.

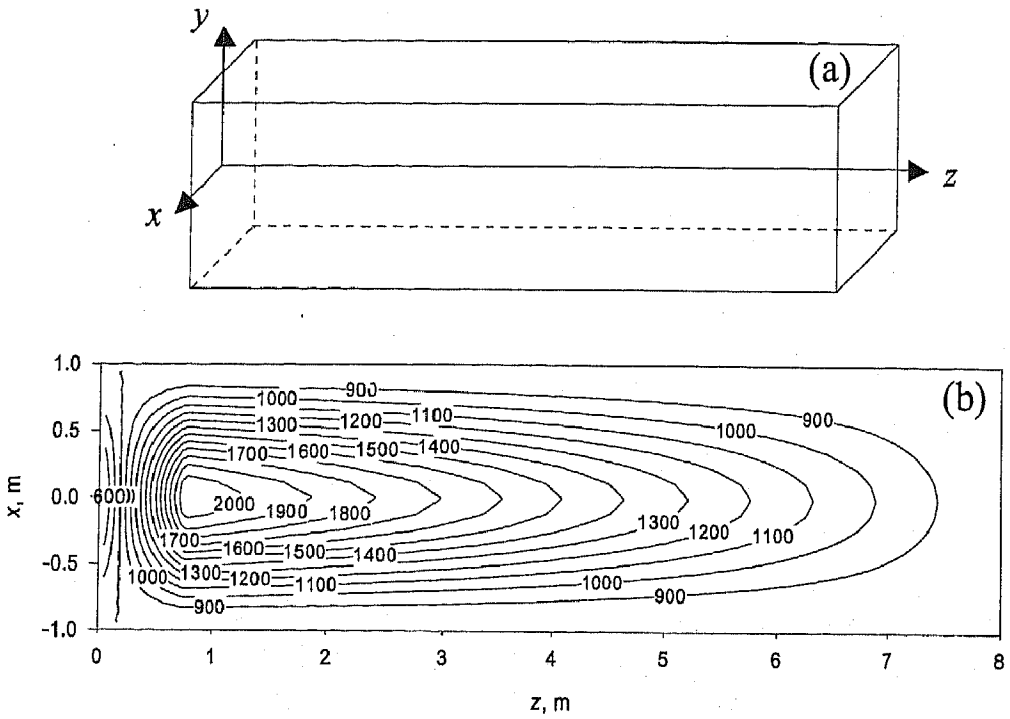

Figure 2. Schematic of the three-dimensional rectangular enclosure, (a), and the temperature distribution in the x-z plane at $y = 0$, (b)

Homogeneous distributions of CO_2 and H_2O The mole fraction distributions of CO_2 and H_2O in this case are uniform at 0.1 and 0.2, respectively. The calculated distributions of wall heat flux along the center of the side wall and the divergence of heat flux along the centerline of the enclosure using the SNB-FSCK methods are compared with those from the SNB-CK method in Fig. 3. Results of the SNB-FSCK/M1 (using the first treatment method for mixture) method are in excellent agreement with those of the standard SNB-CK method, implying that the first method of handling mixtures of CO_2 and H_2O is quite accurate and the choice of the reference temperature T_0 as determined from Eq.(18) is adequate. Results of the correlated treatment for mixture of CO_2 and H_2O, SNB-FSCK/M2, are in significant error, with the relative errors at the maximum absolute values of heat flux and divergence being about 15% and 14%, respectively. Results of the optimized 9-band model, on the other hand, are quite accurate with the relative errors at the maximum absolute values of heat flux and divergence being only about 2%. It is interesting to observe that both the SNB-FSCK/M2 and the SNB-CK/9band model assume that the absorption coefficients of CO_2 and H_2O are correlated. The difference is that in the former the assumption of correlation is made in the full-spectrum and in the latter the assumption is made only at each wide band. Results shown in Fig.3 indicate the main source of error of the second treatment of mixture lies in the assumption of the correlation of the full-spectrum absorption coefficients of CO_2 and H_2O, i.e Eq.(17) yields the mixture absorption coefficients with large error. On the other hand, the assumption of the correlation between the absorption coefficients of CO_2 and H_2O at wide bands, such as in the SNB-CK/9band model, does not introduce significant errors.

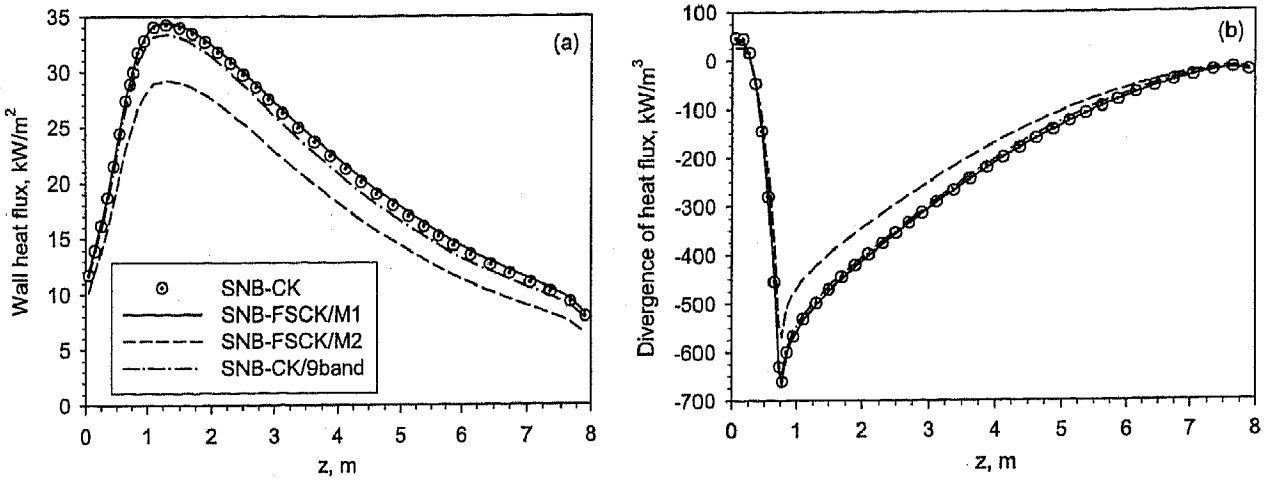

Figure 3. Distributions of heat flux along the center of the side wall, (a), and the divergence of heat flux along the centerline of the enclosure, (b), for homogeneous CO_2 and H_2O mole fractions

Inhomogeneous distributions of CO_2 and H_2O In the second test case, the distributions of mole fractions of CO_2 and H_2O are linear in z-direction and uniform in x and y directions. The mole fraction of CO_2 is assumed as 0 at z = 0, 0.3 at z = 0.5 m, 0.05 at z = 8 m, and varies linearly between these three locations. The mole fraction of H_2O is similarly defined as 0 at z = 0, 0.5 at z = 0.5 m, 0.05 at z = 8 m, and again varies linearly between three locations. Distributions of wall heat flux along the center of the side wall and the divergence of heat flux along the centerline of the enclosure are compared in Fig. 4. Results of the SNB-FSCK/M1 method are again in very good agreement with those of the SNBCK method in this non-isothermal and inhomogeneous case. The correlated treatment for overlap of CO_2 and H_2O in the full-spectrum, SNB-FSCK/M2, again results in significant error, with the relative errors at the maximum absolute values of heat flux and divergence being about 11% and 18%, respectively. Once again, the optimized 9-band model (SNB-CK/9band) predicts quite accurate heat flux and divergence of heat flux with the relative errors at the maximum absolute values of heat flux and divergence being only about 5% and 6.5%, respectively.

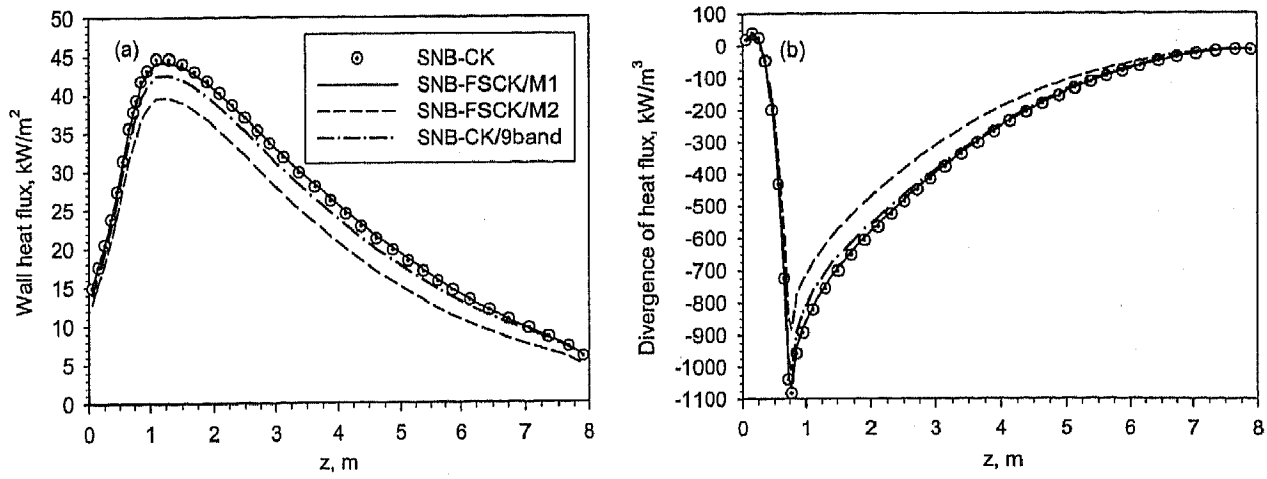

Figure 4. Distributions of heat flux along the center of the side wall, (a), and the divergence of heat flux along the centerline of the enclosure, (b), for inhomogeneous CO_2 and H_2O mole fractions

Comparison of computational efficiency The cpu times of the standard SNB-CK method, the two SNB-FSCK methods, and the optimized 9-band model in the calculation of the above two test cases are compared in Table 1.

Table 1
Comparison of cpu times

Methods	No. of quadrature points	No. of bands	cpu time, s
SNB-CK	7	367	9086.3
SNB-FSCK/M1	4	1	146.9
SNB-FSCK/M2	4	1	30.7
SNB-CK/9band	4	9	84.91

Although the cpu time of the SNB-FSCK/M1 method is significantly lower than that of the standard SNB-CK method by a factor of about 60, such a cpu time reduction is far less than the expected factor of 209 (367×4/7), suggesting that inversion of the cumulative distribution consumes a significant portion of the total time. Compared to the cpu time of the SNB-FSCK/M1 method, use of pre-calculated absorption coefficients of CO_2 and H_2O with correlated treatment for overlap produces a significant savings of cpu time (nearly a factor of 5) but also with significant loss of solution accuracy. Although the RTE needs to be solved over 9 bands (instead of one) in the optimized 9-band model, it is interesting to see that the optimized 9-band model requires significantly less cpu time than SNB-FSCK/M1 (nearly half) and requires only about 2 times more cpu time than SNB-FSCK/M2. This is because the inversion of the cumulative distribution function and the calculation of the weight function a require substantial computing time relative to that spent on DOM. It should be noted that the cpu times compared in Table 1 are for the two specific problems considered in this study, i.e. black walls and therefore no iterations are required. In situations where the boundary walls are grey and the solution must be obtained iteratively, the SNB-FSCK/M1 method may become more efficient than the optimized 9-band model.

Based on the results shown in Figs.3 and 4 and the cpu times in Table 1, it is observed that the SNB based FSCK methods do not offer significant advantages over the optimized 9-band model in terms of efficiency and accuracy. Further more, the optimized 9-band model is capable of accounting for non-grey particulates and boundaries, an advantage that the SNB based FSCK methods cannot

CONCLUSIONS

The statistical narrow-band model based correlated-k method was extended to full-spectrum using the full-spectrum correlated-k methodology. Two methods were proposed to deal with the mixture of CO_2 and H_2O. When using the approximate Malkmus band model for mixture, results of the SNB-FSCK method are almost as accurate as the standard SNB-CK method implemented at narrow-band (25 cm^{-1}) level in the two test cases. Use of pre-calculated absorption coefficients of CO_2 and H_2O and the assumption of correlation between their full-spectrum absorption coefficients reduces the total cpu time of the SNB-FSCK method, but also significantly reduces the solution accuracy. The optimized 9-band model is only slightly less accurate than the SNB-FSCK method with the approximate Malkmus band approach for mixture with better or comparable efficiency. The optimized 9-band offers the best compromise among efficiency, accuracy, and ability to account for non-grey particulates and boundaries and is recommended for radiation heat transfer in multidimensions.

REFERENCES

1. Goody, R., West, R., Chen. L., and Crisp, D., The Correlated-k Method for Radiation Calculations in Nonhomogeneous Atmospheres, *J. Quant. Spectros. Radiat. Transfer*, Vol. 42, No. 6, pp. 539-550, 1989.

2. Lacis, A. A., and Oinas, V., A Description of the Correlated k Distribution Method for Modeling Nongray Gaseous Absorption, Thermal Emission, and Multiple Scattering in Vertically Inhomogeneous Atmospheres, *J. Geophysical Res.*, Vol. 96, No. D5, pp. 9027-9063, 1991.

3. Marin, O., and Buckius, R. O., Wideband Correlated-k Method Applied to Absorbing, Emitting, and Scattering Media, *J. Thermophysics Heat Transfer*, Vol. 10, No. 2, pp. 364-371, 1996.

4. Marin, O., and Buckius, R. O., Wide Band Correlated-k Approach to Thermal Radiative Transport in Nonhomogeneous Media, *ASME J. Heat Transfer*, Vol. 119, pp. 719-729, 1997.

5. Liu, F., Smallwood, G. J., and Gülder, Ö. L., Radiation Heat Transfer Calculations Using the SNBCK Method, *AIAA paper* 99-3679, 1999.

6. Liu, F., Smallwood, G. J., and Gülder, Ö. L., An Accurate Efficient and Flexible SNBCK-Based Unified Band Model for Calculations of Spectrally resolved and Integrated Quantities in Participating Media Containing Real-Gases, *Proceedings of the Twelfth International Heat Transfer Conference*, 663-668, 2002.

7. Denison, M. K., and Webb, B. W., A Spectral Line-Based Weighted-Sum-of-Grey-Gases Model for Arbitrary RTE Solvers, *ASME J. Heat Transfer*, Vol. 115, pp. 1004-1012, 1993.

8. Denison, M. K., and Webb, B. W., The Spectral Line-Based Weighted-Sum-of-Grey-Gases Model in Non-Isothermal Non-Homogeneous Media, *ASME J. Heat Transfer*, Vol. 117, pp. 339-365, 1995.

9. Solovjov, V. P., and Webb, B. W., SLW Modeling of Radiative Transfer in Multicomponent Gas Mixtures, *J. Quant. Spectros. Radiat. Transfer*, Vol. 65, pp. 655-672, 2000.

10. Solovjov, V. P., and Webb, B. W., An Efficient Method for Modeling Radiative Transfer in Multicomponent Gas Mixtures with Soot, *ASME J. Heat Transfer*, Vol. 123, pp. 450-457, 2001.

11. Rivière, PH., Soufiani, A., Perrin, M. Y., Riad, H, and Gleizes, A., Air Mixture Radiative Property Modelling in the Temperature Range 10,000-40,000 K, *J. Quant. Spectros. Radiat. Transfer*, Vol. 56, No. 1, pp. 29-45, 1996.

12. Pierrot, L., Rivière, P., Soufiani, A., and Taine, J., A Fictitious-Gas-Based Absorption Distribution Function Global Model for Radiative Transfer in Hot Gases, *J. Quant. Spectros. Radiat. Transfer*, Vol. 62, pp. 609-624, 1999.

13. Modest, M. F., and Zhang, H., The Full-Spectrum Correlated-k Distribution for Thermal Radiation Distribution for Thermal Radiation from Molecular Gas-Particulate Mixtures, *ASME J. Heat Transfer*, Vol. 124, pp. 30-38, 2002.

14. Zhang, H., and Modest, M. F., A Multi-Scale Full-Spectrum Correlated-k Distribution for Radiative Heat Transfer in Inhomogeneous Gas Mixtures, *J. Quant. Spectros. Radiat. Transfer*, Vol. 73, pp. 349-360, 2002.

15. Zhang, H., and Modest, M. F., Scalable Multi-Group Full-Spectrum Correlated-k Distributions for Radiative Transfer Calculations, *ASME J. Heat Transfer*, Vol. 125, pp. 454-461, 2003.

16. Modest, M. F., Narrow-Band and Full-Spectrum k-Distribution for Radiative Heat Transfer - Correlated-k vs. Scaling Approximation, *J. Quant. Spectros. Radiat. Transfer*, Vol. 76, pp. 69-83, 2003.

17. Goutière, V., Liu, F., and Charette, A., An Assessment of Real-Gas Modelling in 2D Enclosures, *J. Quant. Spectros. Radiat. Transfer*, Vol. 64, pp. 299-326, 2000.

18. Soufiani, A. and Taine, J., High Temperature Gas Radiative Property Parameters of Statistical Narrow-Band Model for H_2O, CO_2 and CO, and Correlated-K Model for H_2O and CO_2, *Int. J. Heat Mass Transfer*, Vol. 40, No. 4, pp. 987-991, 1997.

19. Modest, M. F., and Bharadwaj, S. P., Medium Resolution Transmission Measurements of CO_2 at High Temperature, *J. Quant. Spectros. Radiat. Transfer*, Vol. 73, pp. 329-338, 2002.

20. Liu, F., and Smallwood, G. J., An Efficient Approach for the Implementation of the SNB Based Correlated-k Method and its Evaluation, *J. Quant. Spectros. Radiat. Transfer*, in press.

21. Modest, M. F., *Radiative Heat Transfer*, McGraw-Hill, New York, 1993.

22. Liu, F., Smallwood, G. J., and Gülder, Ö. L., Application of the Statistical Narrow-Band Correlated-k Method to Non-Grey Gas Radiation in CO_2-H_2O Mixtures: Approximate Treatments of Overlapping Bands, *J. Quant. Spectros. Radiat. Transfer*, Vol. 68, pp. 401-417, 2001.

23. Liu, F., Smallwood, G. J., and Gülder, Ö. L., Application of the Statistical Narrow-Band Correlated-k Method to Low-Resolution Spectral Intensity and Radiative Heat Transfer Calculations—Effects of the Quadrature Scheme, *Int. J. Heat Mass Transfer*, Vol. 43, pp. 3119-3135, 2000.